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Air Quality Diffusion Model; Application to New York City

Abstract: An experimental multisource air pollution diffusion model based on the Gaussian plume formulation is described. The model incorporates point and area sources, time and space dependence of source strengths, and time and space dependence of meteorological variables. Numerical simulation of the SO_2 concentration distribution for New York City on January 11, 1971, agrees favorably with experimental measurements.

Introduction

The Palo Alto Scientific Center is developing an experimental "Gaussian plume" diffusion model for the prediction of air pollution concentrations. This model consists of a set of mathematical equations that can be solved on a digital computer for given rates of emission of pollutants into the atmosphere under a given set of meteorological conditions, principally wind vectors and atmospheric stabilities. The solution is a set of numerical values giving the concentration of a pollutant such as sulphur dioxide at spatial points in the region under consideration. Mixing and dilution in a diffusion model are ascribed to the random movement of turbulent eddies in the atmosphere, which carry the pollutants along with them. The rate at which this transport and diffusion take place is determined principally by wind speed, temperature gradient, and local topographic conditions.

The equations representing the model are partly phenomenological because some of the parameters must be evaluated from experimental observations. The use of such a model requires weather and pollution data from a real-time monitoring network and a complete catalogue of pollution emissions within the area (the "source emission inventory"). After the parameters in the model are evaluated using real data, the model must be run for a reasonable period of time for "validation," i.e., comparison of the predictions with the subsequent observations.

Turner[1] was the first to develop a multisource diffusion model for an urban area. The various diffusion models that had been developed up to 1968 have been

critically reviewed by Moses[2] and Neiburger[3]. More recent models are the "Air Quality Display Model" developed by the TRW Systems Group[4], the Metropolitan New York Model" by Shieh[5], and the "Practical Multipurpose Urban Diffusion Model for Carbon Monoxide" by Johnson et al.[6].

Gaussian plume model

• General discussion

The physical process that transports the molecules of pollutant from one point to another is principally eddy diffusion, or turbulence, on a much smaller scale than the large-scale fluid motions of the mixing atmosphere. Turbulence generally refers to a collective random (or nearly random) motion involving a group of many molecules.

The description of diffusion of pollutants by turbulence, which is physically related to the temperature stratification of the atmosphere and to the wind field, leads to the concept of stability classes. The stable layers are those located in regions in which large-scale turbulence is suppressed, but small-scale turbulence, or eddy diffusion, still occurs. A mathematical theory of diffusion exists in which the parameter that measures the rate at which diffusion takes place is directly related to the scale and intensity of the turbulence that occurs. The theory is far from complete—many fundamental questions remain unanswered, but it is complete enough to

be applied in a phenomenological sense inasmuch as the parameters that cannot be determined *a priori* can be estimated from experimental results. Such a diffusion theory can then be used, in conjunction with a description of the motion of the wind, to calculate the spread of pollutants through the atmosphere. At this point the theory is empirical, since it contains experimentally estimated parameters, and crude, because it can include the complicated geometry of the real world (buildings, mountains, etc.) in only a generalized sense.

With these qualifications in mind, however, it turns out that the diffusion models under static weather conditions, if carefully applied, can give good order-of-magnitude (and sometimes better) estimates of spatial distributions of time-dependent pollutant concentrations. The estimate can be made on either a short-term or a climatological basis. The diffusion model applied with day-to-day local weather forecasts is more useful in determining the normal background exposure of the population to pollution and the actual onset of an episode. One could even estimate the emission reductions necessary to suppress the episode or identify the major contributors to the concentration of pollutant at any given point.

One of the most accepted computational approaches is the Gaussian plume model for a single fixed source (see, e.g., Ref. 7). A Gaussian plume model assumes that if a pollutant is emitted from a point source, the resulting concentration in the atmosphere, when averaged over sufficient time, will approximate a normal statistical distribution in space. This is a good approximation for sufficiently long time averages. Thus the diffusion of airborne material can be described in terms of a set of diffusion coefficients that correspond to the standard deviation term in the Gaussian function. These coefficients are assumed to be functions of the atmospheric conditions and the distance downwind from the source. In addition, the entire diffusion cloud is assumed to be transported downwind while the cloud diffuses and spreads. Knowing the diffusion coefficients, one can calculate the steady state concentration associated with emission from an elevated, continuous-emission, point source for a given point in space by using the Gaussian plume formula (illustrated in Fig. 1). In general, the Gaussian plume formulation can be applied to the continuous-emission line and area sources, thereby making possible the construction of an urban diffusion model capable of handling sources of various types.

The Gaussian plume model requires three basic inputs when applied to multiple sources:

1. the spatial and temporal variation of the source emissions;
2. the prevailing average wind speed and direction; and
3. the time and space scales over which the pollutants are to be predicted.

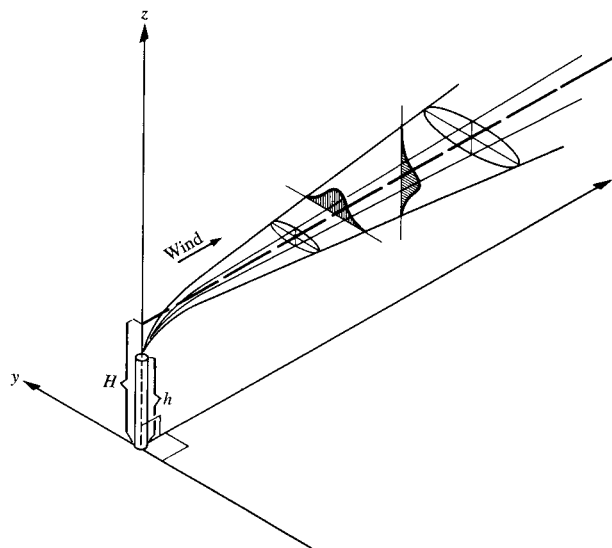


Figure 1 Representation of a continuously emitting point source in the Gaussian plume diffusion model; the function plotted is $\chi\bar{u}/Q$ [see Eq. (1)].

A simulation of concentration fields resulting from multiple sources becomes tractable if one assumes a steady state solution to the diffusion equation for a point source, which has the form of the Gaussian distribution function. By a superposition of single-source solutions, one can represent multiple sources that are spatially distributed and continuous in time.

• Basic equations

The surface concentration field $\chi(x,y,0)$, resulting from a fixed point source at effective height H emitting a gaseous pollutant at the rate Q , can be computed with the formula

$$\chi = \frac{Q}{\pi\bar{u}\sigma_y\sigma_z} \exp - \frac{1}{2} \left(\frac{y^2}{\sigma_y^2} + \frac{H^2}{\sigma_z^2} \right), \quad (1)$$

where the x and y axes are the downwind and crosswind directions, respectively, $\bar{u}$ is the average wind speed, and $\sigma_y(x)$ and $\sigma_z(x)$ are the horizontal and vertical diffusion coefficients. (For a discussion see Ref. 8.) The ground surface is assumed to be a perfect reflector of the pollutants. The effective stack height H has to include the distance the plume rises due to buoyancy; i.e., $H = h + \Delta h$, where h is the physical stack height of the point source and Δh is the plume rise (Fig. 1). In general, Δh can be related to various stack parameters, such as physical configuration of the stack, exit velocity of the flue gas, heat emission rate Q_h , temperature difference between the flue gas at the top of the stack and the ambient air, mean wind speed $\bar{u}$, and local topography. We

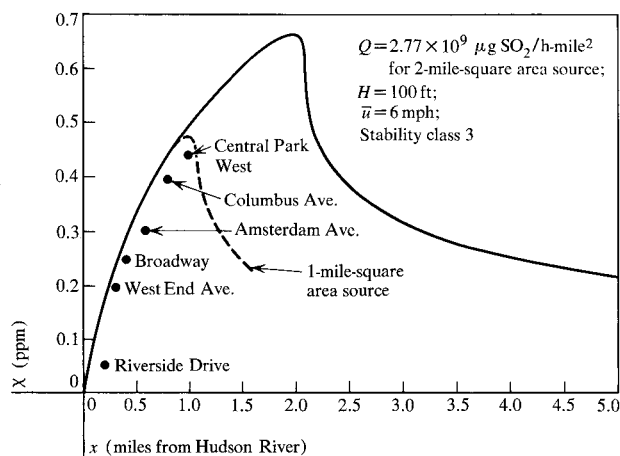


Figure 2 Comparison of observed and computed sulphur dioxide concentrations along 79th Street in New York City for March 9, 1966, 0615 to 0825 EST.

use one of the more widely accepted empirical formulas[9],

$$\Delta h = k Q_h^r / \bar{u}^s, \quad (2)$$

where k , r , and s are experimentally determined constants. (Currently we are using $k = 0.047$, $r = 0.5$, and $s = 0.78$.)

It is not practical to construct a diffusion model for a large region which includes many small sources by treating all of the pollution sources as point sources. To make the computation one combines the small sources within a chosen area into an "area source" with a uniform emission rate. In our model we adopt the integrated plume formula. The concentration at a given point x, y contributed by an area source is obtained by integrating Eq. (1) over the source region:

$$\chi = \int_{y'=-a}^a \int_{x'=0}^{2a} \frac{Q'}{\pi \bar{u} \sigma_y \sigma_z} \exp \left\{ -\frac{1}{2} \left[\frac{(y-y')^2}{\sigma_y^2} + \frac{H^2}{\sigma_z^2} \right] \right\} dx' dy', \quad (3)$$

where σ_y and σ_z are functions of $x - x'$ and the atmospheric stability class, and Q' is the source strength per unit area. In the integration of Eq. (3) the area sources are oriented according to the mean horizontal wind direction.

Figure 2 shows an early use of Eq. (3) to calculate concentration from a continuous area source in New York City. The agreement with observational data is remarkably good. In particular, the ability to simulate the spatial gradient of concentration over a wide range of values portends great promise for using this method, which provides desired accuracy while improving computational efficiency. A detailed discussion of this method compared to other approaches currently used in diffusion modeling is given by Shieh and Halpern[10].

The parameters σ_y and σ_z in Eqs. (1) and (3) are the most controversial in any diffusion equation. It is generally accepted that these parameters depend on atmospheric thermal stability, dynamic wind field, aerodynamic effects of the surrounding boundaries, and travel distance of the plume. The σ curves as functions of plume travel distance are determined by observation for various atmospheric stability conditions and wind speed intervals.

Our model incorporates the σ_y and σ_z values of Pasquill[11] and Gifford[8,12] (especially Ref. 8, pp. 102-103, Figs. 3.10 and 3.11). However, we assume that an inversion layer at height H acts as a barrier to the dispersion of the pollutant so that Gifford's value of σ_z is replaced by σ_z' , where

$$\sigma_z' = \min(\sigma_z, \frac{1}{2}H). \quad (4)$$

• Computational procedure

Given the meteorological and source emission data, the model provides the pollutant concentration at a receptor as the sum of the contributions from the individual sources in the region. The usefulness of this "source-oriented" procedure is twofold. First, one may isolate individually the contribution of any source to the overall concentration field. Second, the procedure is computationally more efficient when the concentration field is to be computed over a relatively large area.

To reduce the computation time for real-time prediction of the concentration fields, an independent program calculates the $\chi \bar{u} / Q'$ function of Eq. (3), which is independent of x' and y' within each source area, for various source sizes, effective stack heights, and atmospheric stability classes. The specification of an inversion layer in the lower atmosphere is also considered as a variable. The results of these computations are stored in a peripheral memory device of the computer.

The main program has four parts: 1) analysis of source inventory data; 2) analysis of meteorological data; 3) calculation of surface pollutant concentration field; and 4) graphic display of computed results. The input requirements for the source inventory and meteorological data are discussed in succeeding sections. The surface pollutant concentration field is determined by the following sequence of computations: 1) area-source contributions; 2) point-source contributions; 3) sum of 1) and 2); 4) 24-hour average of 3).

SO₂ source emission data

The method of producing an inventory of sulphur dioxide emissions for a specific region is well documented. Studies such as those of NAPCA[13], Venezia and Ozolins[14], and Ozolins and Smith[15] describe in detail the procedure for obtaining an annual emission invento-

ry. However, they do not discuss procedures for estimating bihourly emissions from annual emissions for use as input to the air pollution diffusion model.

The diffusion model requires emission data at two-hour intervals in order to predict the average ground level concentration for that period. There are various approaches to obtaining this bihourly data from annual emission data. The method that we outline below has been successfully used in a study by Shieh[5].

In general, the source emissions are usually divided into contributions from industrial sources and from sources that generate space heating and hot water. For modeling, it is inefficient to consider each source as an individual point on the source grid. A logical approach to this problem is to represent all small sources within a reasonable geographic area as a single area source. The individual sources comprising the area source are largely a result of space heating.

The extent of the area sources and their size distribution over the model region are functions of the annual emission inventory and the classification of source types. Table 1 illustrates a typical classification of sources (the definition is not comprehensive).

The area-source and point-source emission data include the location of the sources with respect to a reference coordinate system. This system is defined in the model as a rectangular coordinate system with the origin located at the southwest corner of the geographic region of interest. The x axis represents east-west directions, the y axis, north-south directions, and the z axis, the vertical direction. The x and y coordinates and the physical source height H are required for point sources. The area sources are represented by the geometric center and horizontal extent of the source grid. Each area source grid of a given mesh size has only one source-height parameter H .

• Area sources

Size

The source emission inventory is usually made on a square grid system, using annual data for each grid square. There is no fixed dimension for the mesh size. The techniques used in such a survey are reviewed by Ingram, Kaiser, and Simon[6].

The diffusion model currently accepts various sizes of area source. In areas where SO_2 emission is small, or in areas far from the receptor, the refinement given by a small-mesh grid is not required to obtain a reasonable concentration distribution. In regions of strong SO_2 output, the use of smaller source-grid mesh sizes enables the model to predict concentration fields more accurately. The specification of area sources, i.e., their distribution and dimensions over the model region, is based on the

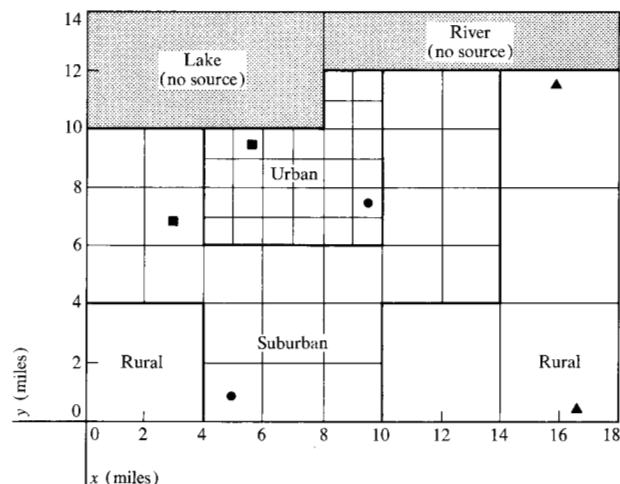


Figure 3 Schematic representation of point sources (● power plant; ■ incinerator; ▲ refinery) and area source grid.

Table 1 Examples of pollutant sources.

Point

Power generator
Incinerator
Manufacturing plant (SO_2 is an indirect product)
Industrial combustion (SO_2 is a direct product)
Chemical refinery
Oil refinery
Mineral smelter
Hospital

Area

Commercial: stores, office buildings, hotels, laundries, etc.
Domestic: space heating, hot water heating, cooking, etc.

receptor location relative to the sources and the distribution of source strengths according to the available source inventory.

The definition of an area source assumes that within the area the emission inventory is approximately uniform. However, it is important to account for any geographic (spatial) gradient of source strength in forming the area source grid map. This map should also reflect large source-free areas such as lakes or rivers. Figure 3 shows a schematic diagram of a typical area source grid map. The one-mile-square mesh is in an urban area where the SO_2 emission is large and the spatial gradient is strong. The two-mile-square mesh is in a suburban area, and the four-mile-square mesh is in a rural area.

Height

The model is capable of handling different source emission heights for each area source mesh size. Since the computational procedure can be made more efficient if

fewer heights are specified, the current model treats only one emission height per area source. The emission height is the average building height within the source area.

Emission rate

One method of subdividing the annual basic area source emission data into two-hour emission periods is to relate daily emission patterns to the average daily temperature. Area source emissions result mainly from fuel combustion for space heating and hot water heating. The amounts consumed are highly dependent on the average daily temperature. Using such a relationship, Ingram et al. [16] suggested the following formula for determining daily output:

$$Q_d = \gamma_1 Q_a / 365 + \gamma_2 DD Q_a / TDD, \quad (5)$$

where Q_d is the daily and Q_a is the annual total output of SO_2 . The degree-day DD is defined as the difference between $65^\circ F$ and the daily mean temperature if the latter is $65^\circ F$ or less; otherwise DD is zero. The long-term climatological average of the annual total degree-days is TDD , and γ_1 and γ_2 are the proportions of sources due to hot water heating and to space heating, respectively ($\gamma_1 + \gamma_2 = 1$).

An alternative to Eq. (5) is based on heating, nonheating, and transient seasons. The calendar year is divided into three specified seasons and the fractions of the annual source emission for these seasons are denoted by α_1 , α_2 , and α_3 , respectively ($\alpha_1 + \alpha_2 + \alpha_3 = 1$). The emission data obtained using this method are not as accurate as those by the former method.

Experience has shown that when the daily mean temperature is greater than $60^\circ F$, there is no significant emission variation in such data. However, different diurnal emission "patterns" are observed when the daily mean temperature lies in the range 30 to $40^\circ F$ or 50 to $60^\circ F$. By assuming that within each $10^\circ F$ interval of the daily average temperature there is a specific pattern of emissions, a simple statistical analysis can be used to obtain 12 two-hour-period coefficients for each temperature range, i.e., the β_i in Eq. (6):

$$Q_i(2h) = \beta_i Q_d, \quad \sum_{i=1}^{12} \beta_i = 1. \quad (6)$$

The accuracy of pollutant concentrations predicted by the model is strongly dependent on the accuracy of the two-hour source emission data.

Small point source in an area source

To reduce the total number of sources handled by the model, we adopt the following criteria for considering a point source as part of an area source: 1) The annual emission from point sources must be less than one tenth of the annual area source emission; 2) the physical stack

height of the point source must be within 20 m of the emission height of the area source; and 3) the point source must have no appreciable plume rise.

Point sources

The sources not classified as area sources are point sources. Associated with point-source input data are the stack parameters mentioned previously as necessary to calculate the rise of the plume above the physical stack height due to buoyancy. Various formulas are available to compute plume rise, e.g., see Ref. 17. One must, however, decide which formula is appropriate for the particular locality. To simplify the computation of plume rise, it is possible to estimate Q_h as a function of $Q(SO_2)$ for each point source or to establish it on an industrial basis.

As in the case of area sources, the model requires bihourly emission data for each of the point sources. If such data are not readily available, the daily emission pattern may be derived from total annual output by classifying the point sources according to industry with an operational mode assigned to each industry. The daily output is assumed to follow a pattern for each industry. For power generation plants, the daily output pattern can be associated with seasonal variation.

The diurnal emission pattern may be formulated analogously to provide the two-hour point source emission data. These are a function of daily output on an industry wide basis. For example, one diurnal emission pattern would be associated with an industry that has a 24-hour operational shift and another pattern would characterize an eight-hour operational shift.

Meteorological data

The diffusion model requires observations of wind speed and direction, averaged over two-hour periods, with a spatial density of observation points dependent on local geography and the observed concentration field. The meteorological data network should be sufficiently dense for a meteorological grid to be defined. (This grid is not necessarily the same as the source grid.) Since the meteorological stations do not necessarily coincide with the grid line intersections, data must be interpolated between the observation points and the meteorological grid, which requires knowledge of the x and y coordinates of the observation locations with respect to the source grid system.

The diffusion model computation uses the atmospheric stability classes defined by Pasquill [11] and used by Turner [1]. These stability classes are based on the vertical thermal stratification. The model requires a stability classification for each two-hour interval.

It is quite common for the region to be covered, in whole or in part, by an above ground temperature inver-

sion layer. The height of this inversion, if present, is included in the input data.

Example

The simulation experiments discussed in this section demonstrate the capability of the diffusion model. Figure 4 is a map of the New York City area showing the locations of the air quality and meteorological observation stations in a four-mile-square grid system. Figure 5 shows the source emission inventory grid with about 500 area sources for the New York metropolitan area. The simulation area is 10.5 miles $\times$ 18 miles and the area source mesh sizes are one-half-, one-, and two-mile squares. The effective areas of simulated sources are related to the geographic gradients of emissions. The two-hour-average emissions for the area sources were obtained with the assistance of the New York City Department of Air Resources by using the annual emissions inventory and Eqs. (5) and (6). Point source data were not used in the example.

The simulation period is the 24 hours of January 11, 1971. The choice of this date was based on two considerations: 1) There was a high sulphur dioxide pollution incident, and 2) a low wind speed condition posed a severe test for the computational method of the model. On that day only five of the ten telemetering stations were operating (1,3,5,14, and 18 in Fig. 4), a not unusual situation in an air quality monitoring network. Four of the operating stations are in the simulation area and station 14 is not far outside it.

A simulation of the SO_2 concentration field for the hours 0200 to 0400 eastern standard time (EST) is shown in Fig. 6(a). The wind for the modeled area is from the southwest at 7 mph. The stability class used is 4. The peak concentration occurs on the west side of mid-Manhattan. There is a very steep concentration gradient across the Hudson River. The general isopleth pattern in Brooklyn, Queens, and the Bronx shows elongation of the closed isopleths in a direction parallel to the mean wind direction.

The observations of ground level sulphur dioxide concentration at station 5 in Manhattan and at stations 1 and 3 in the Bronx verify the simulation for these two areas. In Brooklyn (station 18) the simulation indicates a relative maximum. The 0.08 ppm isopleth falls just to the right of the observed 0.09 ppm. However, in Queens at station 14 the simulation underestimates the concentration by a factor of seven. This is due to two factors: the point source emissions and the new housing in the Queens area—for at least four years, the source inventory has not been updated with these contributions.

The 0800 to 1000 EST simulation is shown in Fig. 6(b). The mean wind direction has changed to northwest, the speed to 4.5 mph, and the stability class to 3.

- Manual
- ▲ Telemetering
- National Weather Service
- Air quality data
- Air quality and meteorological data
- Meteorological data

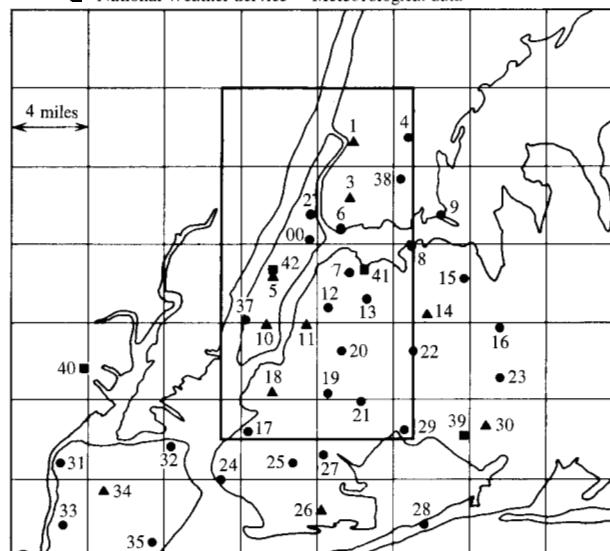
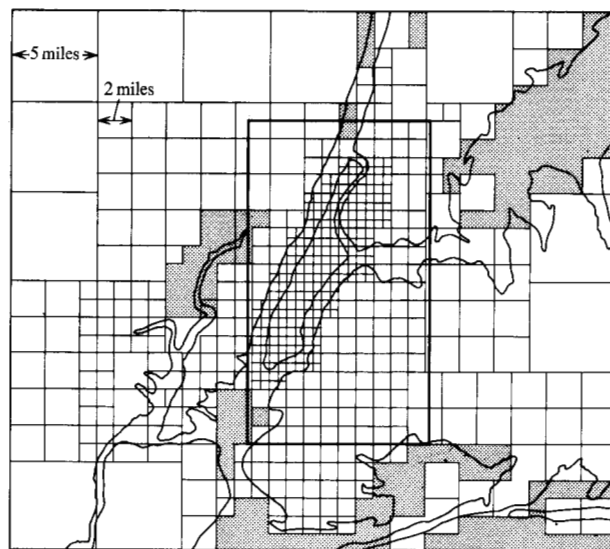


Figure 4 Monitoring stations and meteorological grid. The area simulated in the January 11, 1971, example is outlined in the center.

Figure 5 Area source grid for New York City; the largest mesh is 5 miles square, the smallest, $\frac{1}{2}$ mile square; shading indicates no-source areas.



There are three distinct areas of maximum concentration, two in Manhattan and one in the southeastern Bronx. All three areas are elongated in the direction of the mean wind. The change in wind direction has resulted in the movement of the previous Manhattan maximum from the eastern shore of the Hudson River south-eastward to the East River. A tongue of high concentration extends from the East River into Queens. A second

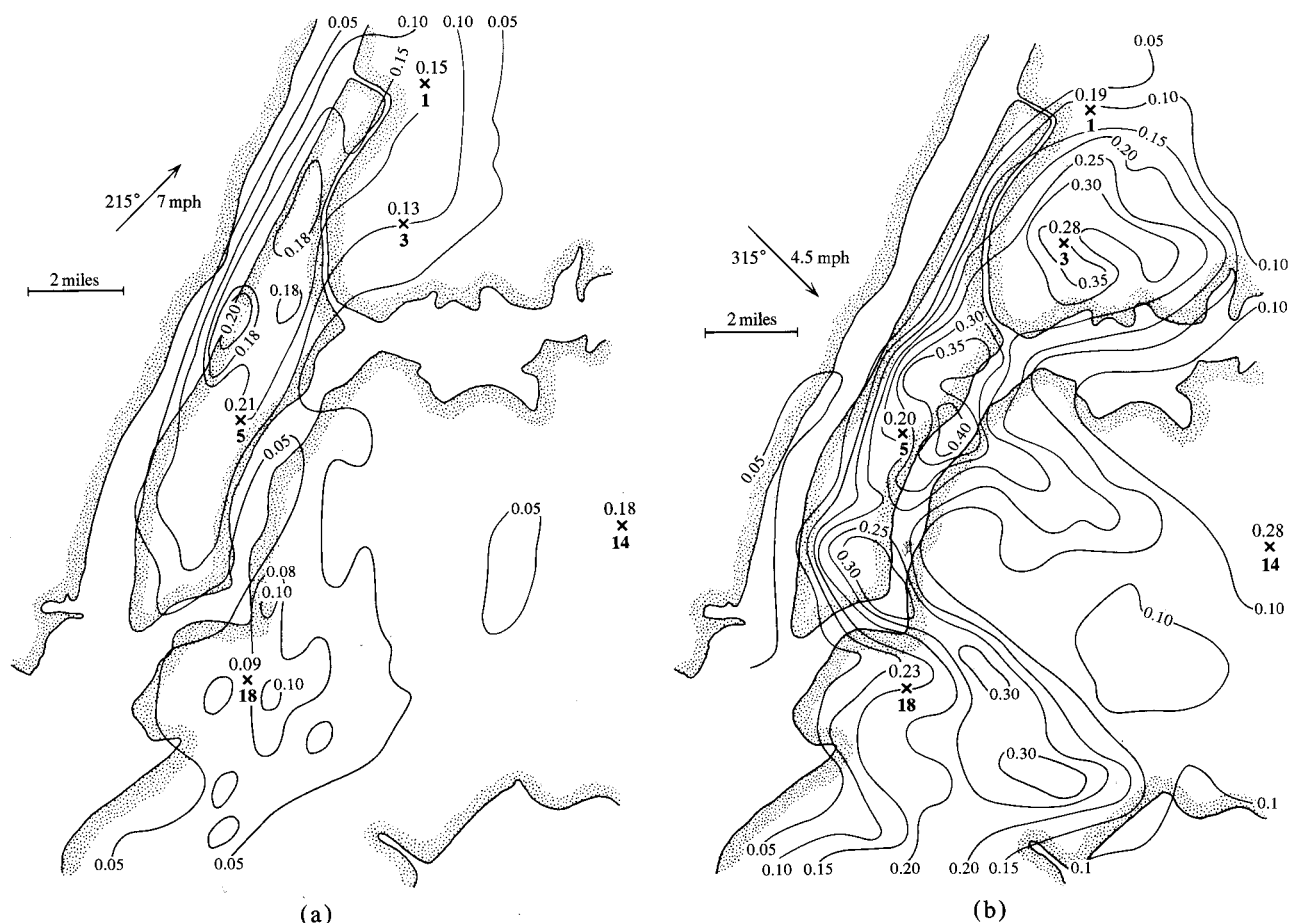


Figure 6 Two-hour simulations of the sulphur dioxide concentration field in New York City on January 11, 1971; observation points and readings are indicated by x: (a) 0200 to 0400 EST, stability class 4; (b) 0800 to 1000 EST, stability class 3.

Table 2 Six- and 24-hour pollutant concentration (ppm) averages for four stations, January 11, 1971.

Time (EST)	Bronx High School (1)		Morrisania Health Center (3)		Central Park Arsenal (5)		Brooklyn Public Library (18)	
	Observed	Computed	Observed	Computed	Observed	Computed	Observed	Computed
0000-0600	0.20	0.19	0.17	0.22	0.22	0.19	0.10	0.09
0600-1200	0.17	0.18	0.14	0.38	0.22	0.24	0.19	0.15
1200-1800	0.14	0.11	0.16	0.18	0.15	0.14	0.09	0.08
1800-2400	0.41	0.30	0.29	0.29	0.25	0.26	0.14	0.14
0000-2400	0.22	0.19	0.22	0.25	0.21	0.21	0.12	0.11

maximum appears in the southeastern part of Manhattan. Here again a region of high concentration extends southeastward to Brooklyn with two relative maxima there. The regions of high concentration are directly related to upwind emissions from areas in Manhattan that have the largest annual emission of SO_2 in all of New York City. The northwest wind has also shifted the early region of maximum SO_2 gradient along the Hudson

River into the western shore line of Manhattan. The observations at stations 1, 3, and 5 verify the simulation quite well. In Brooklyn (station 18) and in Queens (station 14) underestimations by the simulation occur for the reason previously stated.

Figure 7 shows the isopleths of the simulated 24-hour-average surface concentration of SO_2 on January 11, 1971. The peak concentrations occur in Manhattan be-

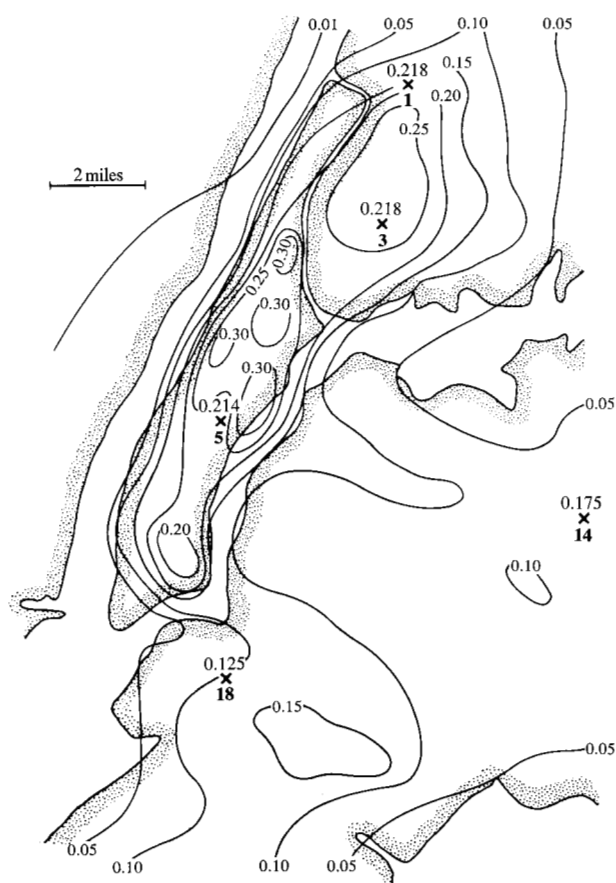


Figure 7 Twenty-four-hour-average simulation of the sulphur dioxide concentration field in New York City on January 11, 1971.

tween station 3 and station 5. A secondary maximum occurs between station 10 and station 37 near the southern end of Manhattan. The southwesterly prevailing wind during the 24-hour period results in a sharp gradient in concentration along the western shoreline of Manhattan. The relatively low-emission sources upwind and the significant density of emission sources downwind (in Manhattan) result in the concentration isopleths' being almost parallel to the shoreline.

The secondary maximum in the southeastern Bronx can be attributed to the high-emission sources in this area and the transport of SO_2 by the wind from Manhattan. There is a large area in Brooklyn and Queens with less than 0.05 ppm concentration. This is also a consequence of the prevailing wind direction and the low emission rate in that area.

The averaged observations of ground level concentration compare favorably with values from the simulation. Station 3 in the southeastern Bronx recorded 0.22 ppm, which is in good agreement with the simulation isopleth of 0.25 ppm. Station 5 in Manhattan agreed with the

0.25 ppm simulation isopleth. The 0.10 ppm isopleth in Brooklyn falls just to the left of station 18, which showed a reading of 0.13 ppm. The simulation in the Queens area near station 14 again underestimated the concentration of SO_2 , thus being consistent with our previous comparisons.

The bihourly variations on January 11, 1971, of the sulphur dioxide concentration are presented in Fig. 8 for four stations. In Table 2, six- and 24-hour averages of the concentrations for the same period are listed for these four stations. In general, there is good agreement between the observed and computed concentration variations for this period.

These numerical experiments indicate that this model has the capability of predicting the general pattern of the ground-level SO_2 concentration in an urban region on a time scale of about two hours. Furthermore, limited comparisons of the simulated values and the observed data in the New York City area give a positive indication of the useful potential of this model. We are presently extending our study to include 1) the spatial dependence of the meteorological input, 2) the point source inventory, and 3) the complete systematic evaluation of the various physical approximations used in the model.

The computer program [18] for this diffusion simulation is written in FORTRAN IV(H) and requires 200K bytes of core storage. For an IBM System/360 Model 91 computer, the CPU execution time for a two-hour simulation was 15 seconds.

Acknowledgments

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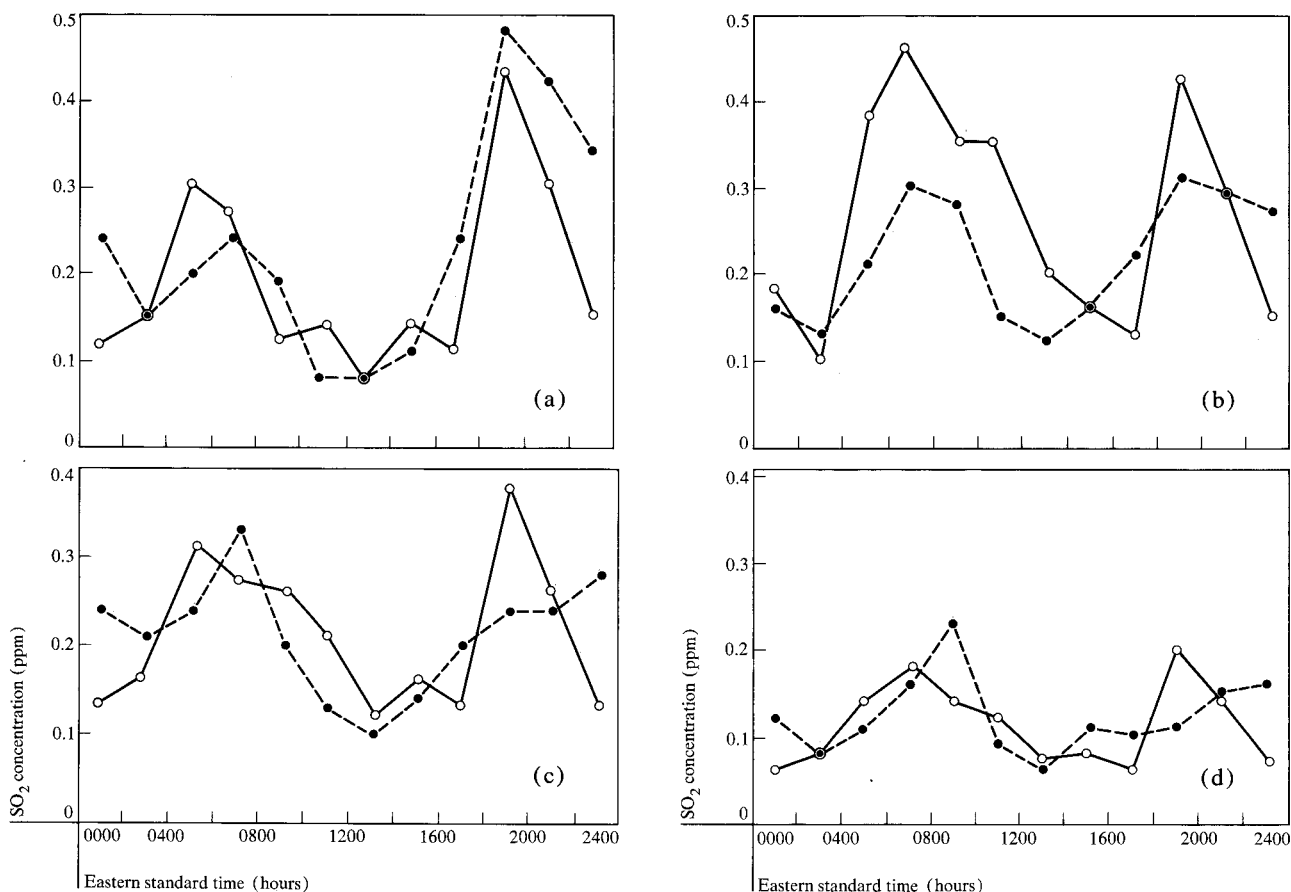


Figure 8 Comparison of the observed (●) and computed (○) bihourly variations of the sulphur dioxide concentration field in New York City on January 11, 1971; (a) station 1, Bronx High School; (b) station 3, Morrisania Health Center; (c) station 5, Central Park Arsenal; (d) station 18, Brooklyn Public Library.

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